WEST Search History

DATE: Wednesday, September 10, 2003

Set Name side by side	Query	Hit Count	Set Name result set
DB=USPT,PGPB,JPAB,EPAB,DWPI,TDBD; PLUR=YES; OP=OR			
L14	L12 same database	6	L14
L13	L12 same optic$4	17	L13
L12	l8 same control$7	735	L12
L11	L9 same computer	14	L11
L10	L9 same optic$4	1	L10
L9	L8 same database	82	L9
L8	(protein or macromolecular) near2 crystal$8	5218	L8
L7	L3 same computer	55	L7
L6	L4 same (voice or spoken or oral)	3	L6
L5	L4 same (voice or spoken or oral)\	3	L5
L4	L3 same computer	55	L4
L3	L2 same optic$3	138	L3
L2	L1 same database	16210	L2
L1	(protein or macromolecular) (2a) crystal$8	1899576	L1

END OF SEARCH HISTORY

SWER 6 OF 33 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:489886 CAPLUS
DN 135:73704
TI Dynamically **controlled** crystal growth system
IN Bray, Terry L.; Kim, Larry J.; Harrington, Michael; Delucas, Lawrence J.
PA University of Alabama, USA
SO U.S. Pat. Appl. Publ., 43 pp., Cont. of U.S. Ser. No. 719,481.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2001006807	A1	20010705	US 1998-131729	19980810
	US 6406903	B2	20020618		
	US 2003027997	A1	20030206	US 2002-85479	20021009
PRAI	US 1995-4267P	P	19950925		
	US 1996-719481	B1	19960925		
	US 1998-131729	A1	19980810		

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     (FILE 'HOME' ENTERED AT 13:42:25 ON 10 SEP 2003)

     FILE 'CAPLUS' ENTERED AT 13:42:37 ON 10 SEP 2003
L1           682 S MACROMOLECUL? (2A) CRYSTAL?
L2         10857 S PROTEIN (2A) CRYSTAL?
L3         11429 S L1 OR L2
L4            97 S L3 AND SOFTWARE
L5           112 S L3 AND DATABASE
L6             1 S L5 AND OPTIC?
L7             0 S L3 AND (DATA (1W) INPUT)
L8             0 S L5 AND (VERBAL OR ORAL OR SPOKEN)
L9            20 S L3 AND (VERBAL OR ORAL OR SPOKEN)
L10           29 S L5 AND COMPUTER

     FILE 'STNGUIDE' ENTERED AT 13:59:42 ON 10 SEP 2003
L11            0 S L3 AND CONTROL?

     FILE 'CAPLUS' ENTERED AT 14:03:10 ON 10 SEP 2003
L12          854 S L3 AND CONTROL?
L13           37 S L12 AND COMPUTER
L14            4 S L13 AND OPTIC?

     FILE 'STNGUIDE' ENTERED AT 14:05:13 ON 10 SEP 2003
L15            0 S L13 NOT L14

     FILE 'CAPLUS' ENTERED AT 14:08:47 ON 10 SEP 2003
L16           33 S L13 NOT L14

     FILE 'STNGUIDE' ENTERED AT 14:14:26 ON 10 SEP 2003

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CODEN: RSINAK; ISSN: 0034-6748
DT Journal
LA English
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB A **computer-controlled** microscopy system for following the face growth of multiple small (.apprx.10-50 .mu.m) crystals during 1 exptl. run is described. The major system components are a **controlling** PC with a digital oscilloscope board, PC-**controlled** translation stages for X, Y, and Z axes of motion, a video microscopy system, and a circuit to trigger digitization of preselected video lines. Crystal locations in the growth chamber are stored in an array, and sequentially accessed during each measurement cycle. Operator-selected horizontal video scan lines are digitized and these data are used to calc. the distance between parallel faces of the crystals. The system was assembled from readily available components, and can be easily modified for other microscopy-based tracking and measuring functions.
ST **computer controlled** microscopy **protein crystal** growth
IT Proteins, properties
RL: USES (Uses)
(**computer-controlled** microscopy system for following crystal face growth rates of)
IT Microscopes
(**computer-controlled**, for following **protein crystal** face growth rates)
IT Crystal growth
(of proteins, **computer-controlled** microscopy system for following face)
IT 9001-63-2, Lysozyme
RL: USES (Uses)
(**computer-controlled** microscopy system for following crystal face growth rates of)

L16 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1987:468624 CAPLUS
DN 107:68624
TI A system for collection and on-line integration of x-ray diffraction data from a multiwire area detector
AU Blum, M.; Metcalf, P.; Harrison, S. C.; Wiley, D. C.
CS Dep. Biochem. Mol. Biol., Harvard Univ., Cambridge, MA, USA
SO Journal of Applied Crystallography (1987), 20(3), 235-42
CODEN: JACGAR; ISSN: 0021-8898
DT Journal
LA English
CC 75-10 (Crystallography and Liquid Crystals)
Section cross-reference(s): 6
AB A system for collecting and measuring x-ray diffraction data from **protein crystals** was developed for a multiwire area detector. The self-contained system consists of an x-ray area detector, a rotation/oscillation camera, and 2 microcomputers connected by a high-speed Ethernet network. One microcomputer is dedicated to operation of the detector, **control** of the camera, and storage of the raw data. The 2nd microcomputer automatically integrates the data as they are collected and allows the user to monitor the quality of data as they are processed. The integration programs are written in Fortran 77 and designed to be portable. Addnl. programs for crystal alignment, detector and camera **control**, and graphics are written in the C programming language. A description of the system, some characteristics of the detector, and the results of data collection are presented.
ST x ray diffraction data processing protein; structure protein x ray diffraction data; **computer** program x ray diffraction protein
IT **Computer** program
(for x-ray diffraction data collecting and redn. from **protein crystals** using multiwire area detector)
IT Crystal structure determination

(of proteins, system for collection and online integration of diffraction data from multiwire area detector in)

IT Proteins, properties
RL: PRP (Properties)
(x-ray diffraction of, system for collection and online integration of data from, using multiwire area detector)

IT Diffractometry
(x-ray, of proteins, system for collection and online integration of data from multiwire area detector)

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L14 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1983:189500 CAPLUS
DN 98:189500
TI Peak-shape analysis for **protein** neutron **crystallography** with position-sensitive detectors
AU Schoenborn, Benno P.
CS Biol. Dep., Brookhaven Natl. Lab., Upton, NY, 11973, USA
SO Acta Crystallographica, Section A: Foundations of Crystallography (1983), A39(3), 315-21
CODEN: ACACEQ; ISSN: 0108-7673
DT Journal
LA English
CC 75-10 (Crystallography and Liquid Crystals)
Section cross-reference(s): 6, 34
AB In neutron **protein crystallog.**, the use of position-sensitive detectors **controlled** by a modern data-acquisition system permits new approaches to data-collection strategies. Instead of dealing with conventional scans, like the .theta.-2.theta. scan, that provide an integrated intensity as a function of a rotational parameter, the **computer**-linked counter can be used to produce a 3-dimensional reflection profile. As the crystal steps (.DELTA..omega.) through a reflection, the obsd. data for each step are stored in an external memory as a function of extent in 2.theta. and height (y) of a reflection. In this space, the reflection will be a 3-dimensional distribution with dimensions detd. by such basic geometrical conditions as .DELTA..lambda., crystal size, mosaic spread, counter-resoln., and beam-collimation parameters. Knowledge of the interaction of these basic parameters will allow the design of optimal beam **optics** and will permit the delineation of the reflection from the background and permit, therefore, an accurate intensity detn.
ST protein structure neutron diffraction
IT Proteins
RL: PRP (Properties)
(crystal structure detn. of, by neutron diffraction, peak shape anal. with position-sensitive detector in)
IT Crystal structure determination
(of protein, by neutron diffraction, peak shape anal. with position-sensitive detector in)

ANSWER 21 OF 29 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1995:770606 CAPLUS

DN 123:164283

TI An integrated x-ray measurement and computation system in **protein crystallography**

AU Fujii, Isao; Hirayama, Noriaki; Morimoto, Yukio; Misaki, Shintaro; Higuchi, Yoshiki; Yasuoka, Noritake

CS Department of Biological Science and Technology, Tokai University, Numazu, 410-03, Japan

SO Bioimages (1994), 2(2), 143-8
CODEN: BIOIFW; ISSN: 0919-2719

PB Bioimaging Society

DT Journal

LA English

CC 9-1 (Biochemical Methods)
Section cross-reference(s): 6, 75

AB A crystallog. workbench or workstation installed with software packages and **database** systems is described, which enables a through processing from x-ray measurement to protein structure anal. As workstations have been installed in many crystallog. labs., a through x-ray anal. system can now be constructed via a local area network. The authors describe the construction of an integrated system for measuring the x-ray intensities from any crystal specimen, transferring structure factor data via the network, carrying out the structure anal., and displaying the mol. structure.

ST **protein crystallog** x ray **computer** system; diffractometry x ray protein computation system

IT **Computer** application
Computer program
Crystal structure determination
(integrated x-ray measurement and computation system in **protein crystallog.**)

IT Proteins, properties
RL: PRP (Properties)
(integrated x-ray measurement and computation system in **protein crystallog.**)

IT Diffractometry
(x-ray, integrated x-ray measurement and computation system in **protein crystallog.**)

L10 ANSWER 29 OF 29 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1988:109167 CAPLUS
DN 108:109167
TI Prediction of protein structure from C.alpha. atomic coordinates
AU Reid, Lorne S.; Thornton, Janet M.
CS Dep. Crystallogr., Birkbeck Coll., London, WC1E 7HX, UK
SO UCLA Symposia on Molecular and Cellular Biology, New Series (1987), 69(Protein Struct., Folding, Des. 2), 93-102
CODEN: USMBD6; ISSN: 0735-9543
DT Journal
LA English
CC 9-15 (Biochemical Methods)
Section cross-reference(s): 6, 75
AB The tertiary structure of flavodoxin was modeled from only its x-ray crystallog. C.alpha.-coordinates. Main-chain atoms were generated from a dictionary of backbone structures. Side-chain conformations were set according to obsd. statistical distributions. Finally, a global energy minimization was applied. The root mean square deviation of the model was 1.7 .ANG. to the native structure. The following parameters were assessed to det. the accuracy of the model: (1) the no. and type of side-chain contacts; (2) water accessibility; and (3) the size of internal cavities. A **database** of side-chain interactions was prepd. to aid in their modeling.
ST protein tertiary structure prediction atomic coordinate; flavodoxin tertiary structure modeling; x ray **crystal** structure **protein**
IT **Computer** program
(for protein tertiary structure prediction from x-ray crystallog. C.alpha. coordinates, PAIRS)
IT Conformation and Conformers
(of proteins, prediction of tertiary structure in, from x-ray crystallog. C.alpha. coordinates)
IT Molecular structure determination
(of proteins, tertiary structure prediction in, from x-ray crystallog. C.alpha. coordinates)
IT Flavodoxins
Proteins, properties
RL: PRP (Properties)
(tertiary structure of, prediction of, from x-ray crystallog. C.alpha. coordinates)

L10 ANSWER 26 OF 29 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1990:563116 CAPLUS
DN 113:163116
TI A menu-driven retrieval system for the **crystallographic database, Protein** Data Bank
AU Sugawara, Yoko; Noguchi, Mamoru; Watanabe, Yasunari
CS Inst. Phys. Chem. Res., Wako, 351-01, Japan
SO Nippon Kessho Gakkaishi (1990), 32(1), 12-19
CODEN: NKEGAF; ISSN: 0369-4585
DT Journal
LA Japanese
CC 75-10 (Crystallography and Liquid Crystals)
Section cross-reference(s): 6, 34
AB The protein data bank maintenance system (PDBMS) was constructed by using Fujitsu's PFD (Programming Facility for Display users) interactive control function on the FACOM M-780 **computer**. This system enables one to search for and retrieve **protein crystallog**. data in the protein data bank by pull-down menus.
ST **protein** data bank **crystallog** data
IT Proteins, properties
RL: PRP (Properties)
(crystallog. **database** for)
IT Information science and technology
(system, computerized, for **protein crystallog**.)

L10 ANSWER 27 OF 29 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1990:194859 CAPLUS
DN 112:194859
TI SIRIUS. An automated method for the analysis of the preferred packing arrangements between protein groups
AU Singh, Juswinder; Thornton, Janet M.
CS Birkbeck Coll., Univ. London, London, WC1E 7HX, UK
SO Journal of Molecular Biology (1990), 211(3), 595-615
CODEN: JMOBAK; ISSN: 0022-2836
DT Journal
LA English
CC 9-15 (Biochemical Methods)
AB Automated methods have been developed to det. the preferred packing arrangement between interacting protein groups. A suite of FORTRAN programs, SIRIUS, is described for calcg. and analyzing the geometries of interacting **protein** groups using **crystallog**. derived at. coordinates. The programs involved in calcg. the geometries search for interacting pairs of protein groups using a distance criterion, and then calc. the spatial disposition and orientation of the pair. The 2nd set of programs is devoted to anal. This involves calcg. the obsd. and expected distributions of the angles and assessing the statistical significance of the difference between the 2. A **database** of the geometries of the 400 combinations of side-chain to side-chain interaction has been created. The approach used in analyzing the geometrical information is illustrated here with specific examples of interactions between side-chains, peptide groups, and particular types of atom. At the side-chain level, an anal. of arom.-amino interactions, and the interactions of peptide carbonyl groups with arginine residues is presented. At the at. level, the analyses include the spatial disposition of O atoms around tyrosine residues, and the frequency and type of contact between C, N and O atoms. This information is currently being applied to the modeling of protein interactions.
ST protein interaction modeling **computer** program
IT **Computer** program
(for protein sidechain interactions anal. using prefered packing arrangements, SIRIUS)
IT Proteins, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(interactions of sidechains of, with other proteins, **computer** programs for anal. of)

6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:23931 CAPLUS
DN 130:88362
TI New crystallization systems envisioned for microgravity studies
AU Bray, Terry L.; Kim, Larry J.; Askew, Raymond P.; Harrington, Michael D.; Rosenblum, William M.; Wilson, W. William; DeLucas, Lawrence J.
CS Center for Macromolecular Crystallography, The University of Alabama at Birmingham, Birmingham, AL, 35294-0005, USA
SO Journal of Applied Crystallography (1998), 31(4), 515-522
CODEN: JACGAR; ISSN: 0021-8898
PB Munksgaard International Publishers Ltd.
DT Journal
LA English
CC 75-1 (Crystallography and Liquid Crystals)
AB Lab.-based systems were constructed to demonstrate two methods which will allow for dynamic **control** of **protein-crystal** growth. The technologies developed in these systems will be incorporated into future flight hardware for use in microgravity studies. The 1st method uses a precisely **controlled** vapor-diffusion approach to monitor and **control protein-crystal** growth. This approach uses a humidity sensor and various interfaces under **computer control** to effect virtually any evapn. rate from up to 40 different growth solns. simultaneously. A static laser-light-scattering sensor can be used to detect aggregation events and trigger a change in the evapn. rate for a growth soln. The 2nd method exploits the varying soly. of proteins vs. temp. to **control** the growth of **protein crystals**. This approach uses miniature thermo-elec. devices under microcomputer **control** which change temp. as needed to grow crystals of a given protein. Complex tempera- ture ramps are possible using this approach. A static laser-light-scattering probe is also included in this system as a noninvasive probe for detection of aggregation events. The systems constructed demonstrate significant advances in the ability of researchers to gain **control** of the **protein-crystal** growth process and will provide tremendous opportunities for microgravity research.
ST crystn system microgravity
IT Hygrometers
(in crystn. systems for microgravity studies)
IT Crystallization apparatus
Microgravity
(new crystn. systems envisioned for microgravity studies)
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Baker, E; J Mol Biol 1970, V54, P605 CAPLUS
(2) Cacioppo, E; J Cryst Growth 1991, V110, P66 CAPLUS
(3) Casey, G; J Cryst Growth 1992, V122, P95
(4) Chayen, N; J Appl Cryst 1990, V23, P297 CAPLUS
(5) Cox, M; J Cryst Growth 1988, V90, P318 CAPLUS
(6) Eisele, J; J Appl Cryst 1993, V26, P92 CAPLUS
(7) Fowlis, W; J Cryst Growth 1988, V90, P117 CAPLUS
(8) Hanson, A; J Biol Chem 1970, V245, P4975
(9) McPherson, A; Biochem Biophys Acta 1972, V285, P493 CAPLUS
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(11) Shotton, D; J Mol Biol 1968, V32, P155 CAPLUS
(12) Smith, H; J Cryst Growth 1991, V110, P137 CAPLUS
(13) Wilson, L; J Cryst Growth 1991, V110, P142 CAPLUS
(14) Wilson, L; J Cryst Growth 1992, V116, P414 CAPLUS

L16 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1994:90294 CAPLUS
DN 120:90294
TI A **computer-controlled** microscopy system for following **protein crystal** face growth rates
AU Pusey, Marc Lee
CS MSFC, NASA, Huntsville, AL, 35810, USA
SO Review of Scientific Instruments (1993), 64(11), 3121-5